

CHEM 4685
Advanced Topics: Spectroscopy
Fall 2019Dr. Megumi Fujita
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Class Period: MW 11:00am-12:15pm **Classroom:** TLC2105
Office hours: M 12:30-3, T 10:30-12:30, W 12:30-2, F 8-10 & 12-2 or by appointment

Pre-Requisite: Completion of CHEM3422 (Organic Chemistry II) with C or higher

Required Course Materials

- **Textbook:** *Organic Structures from Spectra, Fifth Edition* by L. D. Field, S. Sternhell, J. R. Kalman, Wiley, 2013. Obtain a CLEAN copy, as it primarily serves as a workbook.
- Bring **pencils, eraser, ruler, red pen, calculator***, and a **binder & filler notebook sheets** to each class. (*cell phones or electronic devices are NOT allowed)

Course description

Spectroscopy is a vital tool for scientists to gain insight into the substances they study about. This course will focus on structural characterization of molecular compounds using the combination of infrared (IR) spectroscopy, mass spectrometry (MS), ultraviolet (UV) spectroscopy, and nuclear magnetic resonance (NMR) spectroscopy. In addition, you will learn about the analyzed compounds themselves, and see how the molecular structures relate to their physical and chemical properties. The course will include a glance at how spectroscopy is used to in real-world situations (e.g. academic investigation, environmental, forensic, medical, industrial...).

While this course focuses on organic compounds, the study of spectroscopy crosses over into many other fields, including biochemistry, inorganic chemistry, physical chemistry, materials chemistry, and analytical chemistry. Proficiency in spectral analysis is a valuable asset for chemistry majors to pursue any chemistry careers.

Learning outcomes

Upon successful completion of this course, you will know what types of information can be extracted from each type of spectroscopy (MS, IR, NMR and UV), be able to integrate the extracted information to determine the molecular structure of a wide range of organic compounds. You will also be able to assign all the peaks knowing the chemical and physical basis of them (mass fragmentation mechanisms, IR vibration modes, ^1H and ^{13}C NMR chemical shifts and couplings, UV-absorbing electron excitations). You will have a more broaden knowledge of organic compounds and how their structures correlated to their properties. You will be able to propose spectroscopic method(s) suited for the type of analysis needed for a given situation.

<u>Grades</u>	($\geq 90\%$: A $\geq 80\%$: B $\geq 70\%$: C $\geq 60\%$: D $\leq 60\%$: F)
In-class exercises and small homework	15%
Problem set presentations	10%
Compound profiles	5%
Take-home exams (two)	25%
In-class exams (two)	30%
<u>Final exam</u>	<u>15%</u>
Total	100%

- **In-class exercises and small homework:** Some of the in-class exercises and small homework will be collected for grading. Some may be graded in class by the peers following the grading guidelines provided.
- **Problem set presentations:** In many of the classes, problem sets, in the form of handouts or assigned pages in the textbook, will be given. You are expected to have solved all of them by the next class period. Names are drawn randomly to determine who will present which problem. All students will have an equal number of presentations over the semester (estimated 3 rounds, subject to change). These presentations are graded based on the accuracy (correct structure) and thoroughness (all peaks are assigned correctly, and the reason for the assignment can be explained). If you are absent when your name is drawn, a grade of zero will be given for the round.
- **Compound profiles:** After giving a problem set presentation, the presenter will create a “compound profile” about the compound that was identified in the presentation. The compound profile is a 1-page powerpoint to show the structure, name, and some interesting facts (how it is relevant to our lives). Make it visually appealing and informative. The presenter will deposit the file in a shared Google Drive by no later than 10am of the class period after the problem set presentation. The instructor will share them in class, and the creators will be asked to give a 1-minute talk about the compound.
- **Take-home exams:** There will be two take-home exams.
- **Exams:** There will be **two in-class exams** and **one final exam**. You are allowed to bring the textbook, class handouts, your own notes, a simple calculator, and a ruler. No electronic devices are allowed.

Typical class style (it varies day by day)

- 0-5 minutes Compound profiles
- 30 minutes Problem set presentations (6 students) or homework check/peer-grading
- 15-20 minutes new topic
- Rest: In-class exercises
- At the end: homework or problem set will be assigned

How to study for this course

- Actively work on the handouts and the textbook. Write in peak assignments and characterization.
- Don't be afraid to struggle. Train your brain to think like a scientist, who constantly work on unknowns and work hard to find answers. The hard work will be rewarded by the joy of light-bulb moments and true learning.
- Organize the important resources. In the theory pages of the textbook, mark the important tables and charts in a way you can find them quickly. Organize all handouts in a binder for easy access. In-class exams are open-book, but you will need to find needed information quickly.
- Ask questions! Use the office hours! I am here for you to master the materials successfully.
- Work on un-assigned problems on the textbook to practice. This will be a great way to prepare for the in-class and final exams. You can check your answers with the instructor.
- Study group to work on the problem sets can be beneficial. Explaining to each other (or just struggling together) can provide additional perspectives and lead to deeper learning.

Tentative schedule (subject to change)

Week	Dates	Tentative topics	Exam and Take-home dates
1	8/14	Syllabus, tour, IR review	
2	8/19, 21	IR, MS	
3	8/26, 28	MS, MS+IR	
4	9/4	MS+IR	
5	9/9, 11	UV, integrative	Take-home 1
6	9/16, 18	NMR (basics, aromatics), integrative	
7	9/23, 25	NMR (N compounds), integrative	
8	9/30, 10/2	NMR, integrative	10/2 (W) Exam 1
9	10/7, 9	NMR (alkene/alkyne), integrative	
10	10/14, 16	NMR (rings, Karplus), integrative	
11	10/21, 23	NMR (biological & medicinal compounds)	Take-home 2
12	10/28, 30	NMR, integrative	
13	11/4, 6	2D NMR	
14	11/11, 13	2D NMR	
15	11/18, 20	Integrative	11/20 (W) Exam 2
	11/25, 27		
16	12/2, 4	Review (incl. methods, compounds)	
			Final Exam: Wednesday, Dec. 11, 11am-1pm

Locations of the in-class exams: Please note that on the in-class exam days, we will use a different location to allow more space for each student. I'll try my best to find a convenient location in or near the TLC Building. An exam location will be announced in advance.

Other Course Policies

- **Academic integrity** is of prime importance. Any form of dishonesty will be penalized to the fullest extent.
- Use your **MyUWG e-mail** for official correspondence with the instructor. (Do not use the CourseDen email... it will not be read.) Course-related announcements may be made via email and CourseDen course home page, so please check your email often.
- For more information on **academic support, honor code, email policy, credit hour policy** and **HB 280 campus carry policy**, go to: <https://www.westga.edu/UWGSyllabusPolicies/>
- **Cell phones and electronic devices** must be turned off in class and should not be placed in a book bag, or out of sight during the class period. Repeated violation of this policy will result in confiscation of the device for the remainder of the class period, and the reduction of your grade.